WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:02 PM GMT

PDB ID : 1IGC
Title : IGG1 FAB FRAGMENT (MOPC21) COMPLEX WITH DOMAIN III OF PROTEIN G FROM STREPTOCOCCUS
Authors : Derrick, J.P.; Wigley, D.B.
Deposited on : 1994-08-05
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
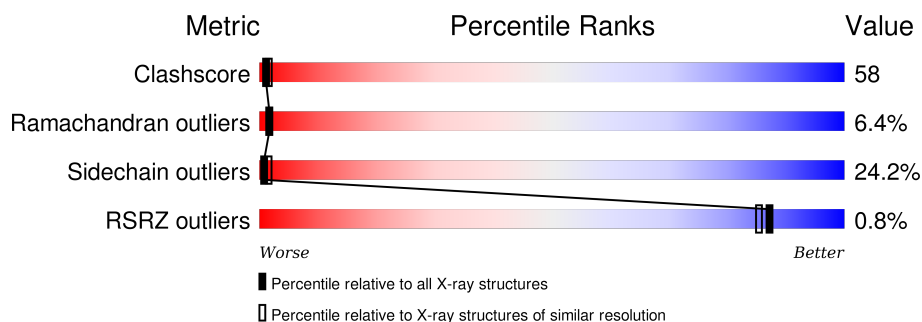
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		58
Ramachandran outliers		6.4%
Sidechain outliers		24.2%
RSRZ outliers		0.8%

Worse ... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	213	23% 41% 26% 9%
2	H	222	27% 44% 21% 8%
3	A	61	30% 48% 13% 5% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IGG1-KAPPA MOPC21 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1651	1025	277	340	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	92	ASN	TYR	CONFLICT	UNP P01634
L	?	-	GLY	DELETION	UNP P01634

- Molecule 2 is a protein called IGG1-KAPPA MOPC21 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1675	1057	281	327	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	VAL	LEU	CONFLICT	UNP P01783
H	13	GLN	LYS	CONFLICT	UNP P01783
H	18	ARG	LEU	CONFLICT	UNP P01783
H	31	SER	ASP	CONFLICT	UNP P01783
H	32	PHE	TYR	CONFLICT	UNP P01783
H	58	LEU	ILE	CONFLICT	UNP P01783
H	59	HIS	TYR	CONFLICT	UNP P01783
H	75	PRO	ALA	CONFLICT	UNP P01783
H	92	GLY	ALA	CONFLICT	UNP P01783
H	?	-	ASP	DELETION	UNP P01783
H	?	-	THR	DELETION	UNP P01783
H	?	-	THR	DELETION	UNP P01783
H	100	GLY	VAL	CONFLICT	UNP P01783
H	101	ASN	SER	CONFLICT	UNP P01783

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Chain	Residue	Modelled	Actual	Comment	Reference
H	102	TYR	GLY	CONFLICT	UNP P01783
H	103	PRO	HIS	CONFLICT	UNP P01783
H	106	ALA	VAL	CONFLICT	UNP P01783
H	194	PRO	THR	CONFLICT	UNP P01783
H	195	ARG	TRP	CONFLICT	UNP P01783
H	198	GLU	GLN	CONFLICT	UNP P01783

- Molecule 3 is a protein called STREPTOCOCCAL PROTEIN G (DOMAIN III).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	A	58	446	280	70	96	0	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	37	37	37	0	0
4	H	145	Total 145	O 145	0	0
4	L	163	Total 163	O 163	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
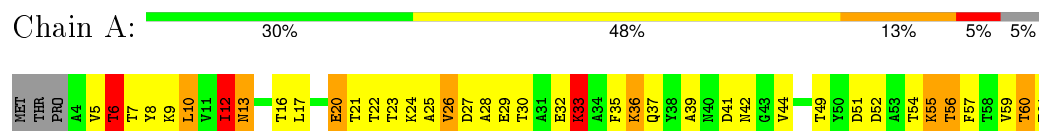
- Molecule 1: IGG1-KAPPA MOPC21 FAB (LIGHT CHAIN)
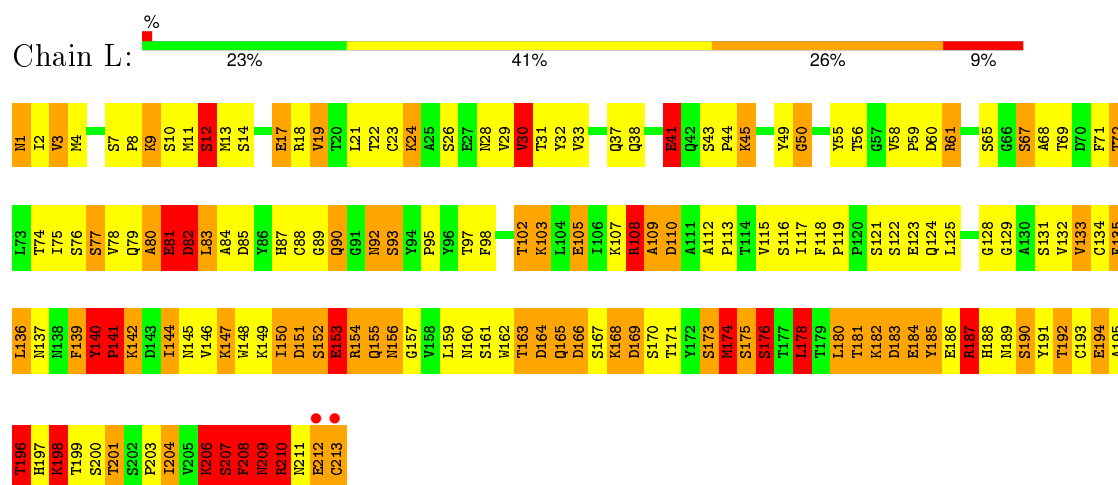
- Molecule 2: IGG1-KAPPA MOPC21 FAB (HEAVY CHAIN)
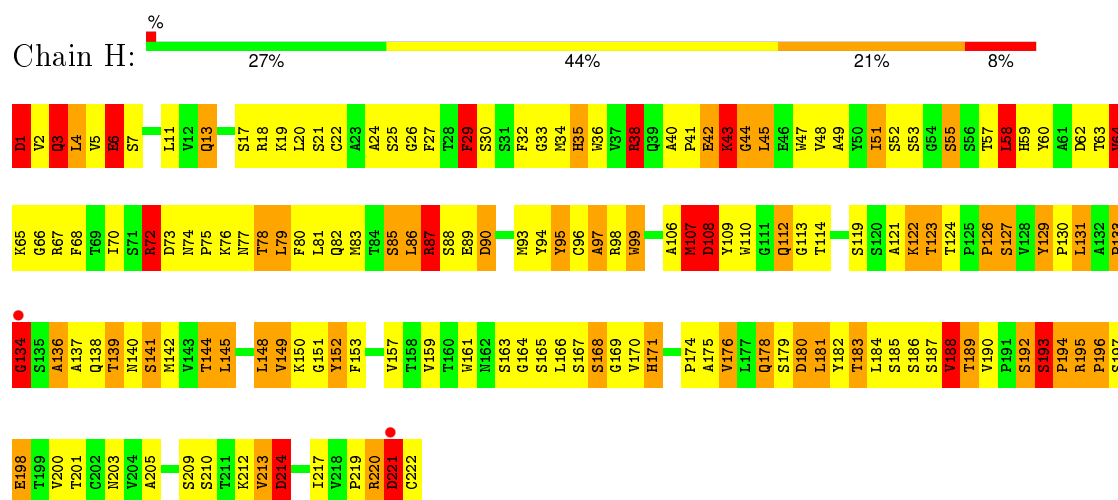
- Molecule 3: STREPTOCOCCAL PROTEIN G (DOMAIN III)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.50Å 70.50Å 120.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 98.7 (19.85-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 2.59Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 188.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 17204 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	L	0.96	2/1687 (0.1%)	2.44	102/2291 (4.5%)
2	H	0.92	0/1722	2.55	92/2352 (3.9%)
3	A	0.87	0/452	2.13	15/613 (2.4%)
All	All	0.93	2/3861 (0.1%)	2.46	209/5256 (4.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	141	PRO	N-CD	6.99	1.57	1.47
1	L	30	VAL	N-CA	5.43	1.57	1.46

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	38	ARG	CD-NE-CZ	29.29	164.60	123.60
2	H	195	ARG	NE-CZ-NH1	27.18	133.89	120.30
2	H	67	ARG	CD-NE-CZ	24.61	158.05	123.60
1	L	141	PRO	N-CA-CB	19.39	126.57	103.30
2	H	195	ARG	CG-CD-NE	18.32	150.27	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1651	0	1575	200	0
2	H	1675	0	1621	200	0
3	A	446	0	433	41	0
4	A	37	0	0	5	0
4	H	145	0	0	18	0
4	L	163	0	0	11	0
All	All	4117	0	3629	431	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 58.

The worst 5 of 431 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:GLN:HE22	2:H:181:LEU:HB2	0.94	1.10
2:H:51:ILE:HD11	2:H:79:LEU:HD13	1.27	1.08
2:H:43:LYS:HG2	2:H:44:GLY:H	0.95	1.08
2:H:43:LYS:CG	2:H:44:GLY:H	1.55	1.08
2:H:193:SER:HB2	2:H:194:PRO:CD	1.83	1.07

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	211/213 (99%)	177 (84%)	18 (8%)	16 (8%)	1	1
2	H	220/222 (99%)	183 (83%)	23 (10%)	14 (6%)	2	2
3	A	56/61 (92%)	53 (95%)	2 (4%)	1 (2%)	11	21
All	All	487/496 (98%)	413 (85%)	43 (9%)	31 (6%)	2	2

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	60	ASP
1	L	82	ASP
1	L	140	TYR
1	L	141	PRO
1	L	150	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	190/190 (100%)	141 (74%)	49 (26%)	0	1
2	H	189/189 (100%)	143 (76%)	46 (24%)	1	1
3	A	47/50 (94%)	39 (83%)	8 (17%)	2	4
All	All	426/429 (99%)	323 (76%)	103 (24%)	1	1

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	211	ASN
2	H	38	ARG
3	A	12	ILE
1	L	212	GLU
2	H	6	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	13	GLN
2	H	35	HIS
2	H	178	GLN
1	L	188	HIS
2	H	112	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	213/213 (100%)	-0.94	2 (0%)	85	83	9, 28, 59, 118	0
2	H	222/222 (100%)	-0.95	2 (0%)	85	83	9, 24, 62, 104	0
3	A	58/61 (95%)	-1.02	0	100	100	14, 30, 45, 71	0
All	All	493/496 (99%)	-0.96	4 (0%)	87	85	9, 26, 60, 118	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	GLU	6.7
1	L	213	CYS	5.8
2	H	221	ASP	2.8
2	H	134	GLY	2.7

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.